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NUMIT-ONE AMENDMENT #1

ARMED FORCES RADIOBIOLOGY RESEARCH INSTITUTE
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NUMIT-ONE AMENDMENT #1

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FOREWORD
(Nontechnical summary)

An improvement in NUMIT-ONE (AFRRI Scientific Report SR65-1, October 1965) is described. Simpson's Rule is still used to perform the integration but changes in the coding remove the need for a large array. The number of multiplication operations done during a run has also been vastly reduced resulting in significant savings in machine time.

ABSTRACT

An improvement on NUMIT-ONE, a one-dimensional numerical integration program for the IBM 1620, is reported. Accuracy, input and output formats, source program, flow charts and test problems are discussed.

I. INTRODUCTION

This is an amendment to NUMIT-ONE, a numerical integration program in one-dimension for the IBM 1620 computer, AFRRI Scientific Report SR65-1. Appendix D contains a glossary of terms used in this report.

Further analysis of the problem resulted in the elimination of a large array thereby making the program smaller and the number of multiplication operations fewer. This reduction in size enabled compilation with a larger precision parameter* (thereby increasing accuracy) and the fewer operations decreased the length of running time.

Successive approximations to the integral are now computed with J successively 1, 2, . . . , using

$$F_J(a,b) = \frac{\Delta X_J}{3}\left[f(a) + f(b) + 2 \cdot C_J + 4 \cdot D_J\right]$$

in which

$$\Delta X_J = \left|\frac{b-a}{2J}\right|$$

$$C_J = \sum_{m=1}^{\frac{2^J}{2}-1} f(a + 2m \cdot \Delta X_J), \quad J > 1; \quad C_J = 0 \text{ if } J = 1$$

$$D_J = \sum_{m=1}^{\frac{2^J}{2}} f(a + [2m-1]\,\Delta X_J)$$

Thus for the J + 1th iteration:

$$C_{J+1} = D_J + C_J$$

---

* A precision parameter is the number of arithmetic places to which quantities will be held during computation and may be specified on a control card that precedes the rest of the deck in IBM 1620 FORTRAN II.

and only two summed quantities in the main equation need be multiplied rather than entire arrays.

Input and output formats are slightly changed from the original version.

II. ACCURACY

Reduced truncation error has improved the accuracy. An inherent weakness in Simpson's Rule makes it difficult or impossible to integrate over the intervals of functions where the slope approaches infinity. In the current version it is still difficult but if a large number of iterations are used and the precision parameter is large enough, an accurate answer will be obtained. Test Case 1 (Appendix C) of the current report illustrates this. The slope of this function approaches infinity at the start and end of this interval. By allowing 11 iterations and holding quantities to 10 places, an answer accurate to 5 places was computed.

Breakdown will definitely occur when the integral is close to zero, resulting from an integrand taking on both positive and negative values over the interval of integration. A function such as this should be integrated in parts.

Input for the program has been changed slightly to make this division of the integration interval more amenable and there are no limits on the number of parts used. This situation reveals itself readily by the erratic behavior of DELTA (Δ_J). Test Case 2 (Appendix C) illustrates what happens when integration is attempted over the whole interval of such an integrand and Test Case 3 illustrates the proper method of splitting the integration into parts.

III. INPUT LIMITATIONS

The integrand, $f(x)$, may be any function for which the integral exists; also $(-\infty) < a, b < (+\infty)$, $b \neq a$.

The total number of iterations allowed is J_{max} (an input parameter) where $2 \leq J_{max} < 100$. Iteration is stopped whenever either

$$\Delta_J \leq \Delta \quad \text{or} \quad J = J_{max}$$

While J_{max} can be any number up to 100, it should not be too high. Each iteration roughly doubles the machine time. Generally, for more than 13 or 14 iterations, machine time is measured in hours.

The integrand, $f(x)$, is provided by a subprogram of the FUNCTION type named FUN(X). FUN must appear on the left of an arithmetic statement whose right is the integrand. The subprogram source deck must be preceded at compilation time by a precision parameter card identical to the precision parameter card, if any was used, of the main source deck.

IV. INPUT AND OUTPUT FORMATS

Input Card Format

The following quantities are specified in the input (floating point numbers are in lower case, fixed point numbers in upper case).

Card 1

Columns 1-80 contain alphanumeric identification. It is reproduced in the output but does not affect the processing.

Card 2

Columns 1-36 Integrand Specification Card. Contains alphanumeric information to identify integrand in output. This does not affect processing.

Card 3

			Format
Columns	1-12	a	E 12.6
Columns	13-24	b	E 12.6
Columns	25-28	Δ	F 4.4
Columns	29-30	J_{max}	I 2

Following card 3 may be any number of cards specifying new values of a, b, Δ, and J_{max}. Input format is the same as card 3. The final card is a trailer card with zeros punched in columns 29-30.

Input Deck Assembly

Input decks are assembled as in the original NUMIT-ONE with the FUN(X) subprogram replacing the POINT subprogram.

Errors in Input

The input error check is the same as before except that in the amended version J_{max} may have any value up to 99. A check is made to see if $J_{max} < 2$.

Output

The output has three main stages; the identification is punched as follows:

(a) Alpha Identification Card

(b) Program name (NUMIT-ONE)

(c) F(X) = Columns 1-36 of Integrand Specification Card.

Next, the input a, b, J_{max}, and DELTA 1 are punched followed by the results of the computation with the following data given for each iteration ($J = 2, \ldots J_{act}$):

(a) Iteration number

(b) Value of integral

(c) DELTA

The final value for DELTA ≤ DELTA 1 or $J_{act} = J_{max}$ is noted by the term (PASS N) in the last line of the output, where N = 1,2...99 is the pass number.

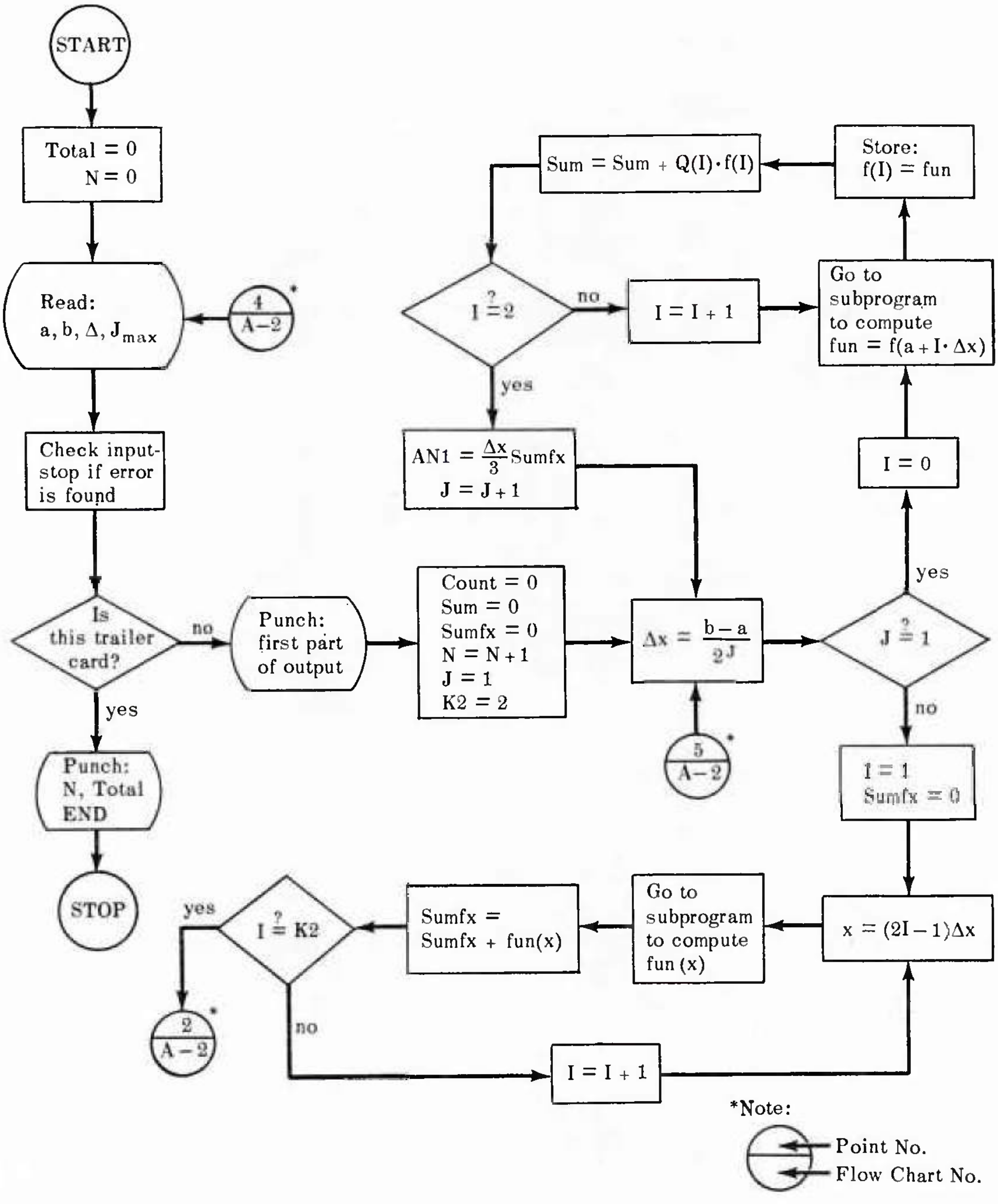
If more cards specifying new values of a, b, J_{max} and DELTA 1 are input, the above cycle will be repeated until all input cards have been processed. The final part of the output is furnished when the trailer card is read. The number of passes (N) is punched, followed by the total value of the integral for all passes. The last card punched, showing satisfactory completion of the program, is "END" and the program stops.

A set of output listings for sample problems is given in Appendix C.

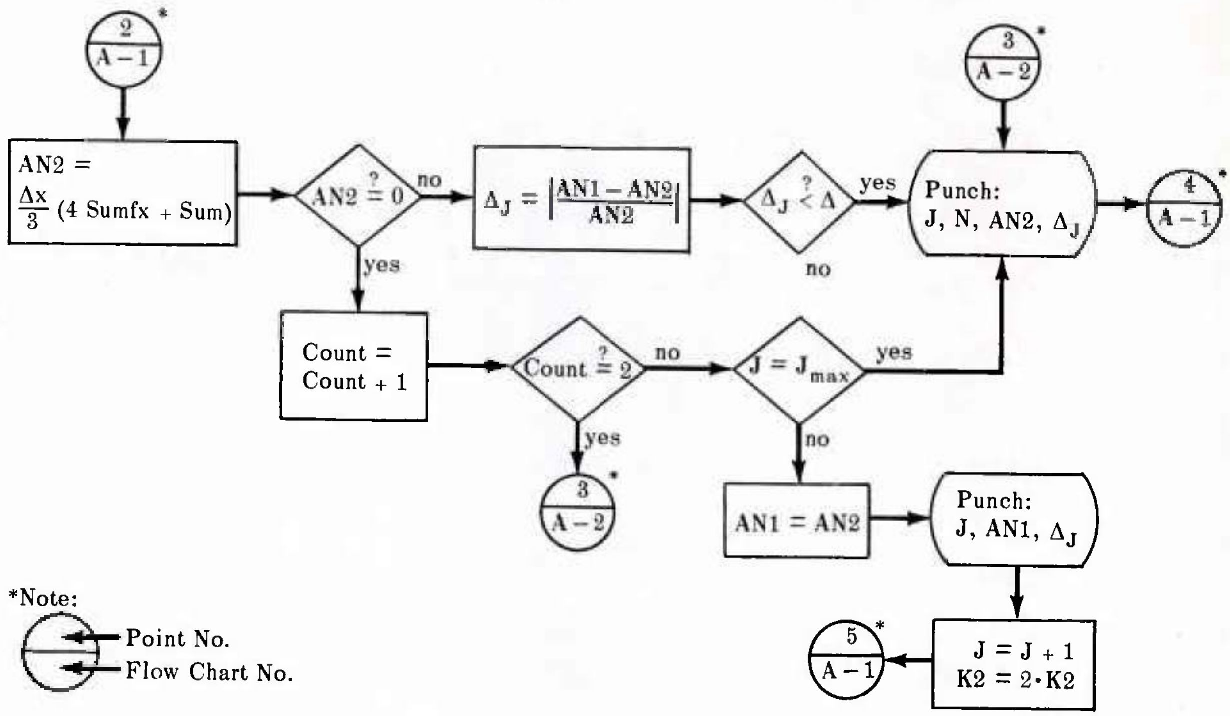
V. OPERATION

Operation is the same as before except a trailer card is now used to stop the computation. No switches are used.

Flow Charts



Flow Chart A-1



Flow Chart A-2

APPENDIX B

<u>Source Program</u>

In the program, the following symbols are used which are unexplained in the mathematical description:

N	=	counter to keep track of number of passes
DELTA 1	=	Δ = input convergence criterion
AN1	=	F_{J-1} = previous approximation
AN2	=	F_J = current approximation
SUMFX	=	$\sum_{m=1}^{2^{J-1}} f(a + [2m-1]\,\Delta x)$
SUM	=	$f(a) + f(b) + \sum_{m=1}^{\frac{2^J}{2}-1} 2 \cdot f(a+2m \cdot \Delta x)$
COUNT	=	counter used to count successive times $F_J = 0$

```
*1010
C       NUMERIC INTEGRATI¤N USING SIMPS¤N- R¤CKWELL-  2-16-66   AFRRI-NNMC
        DIMENSI¤N F(3),P(3),Q(3),U(9)
        P(1)=1.
        P(2)=4.
        P(3)=1.
        Q(1)=1.
        Q(2)=2.
        Q(3)=1.
         N=0
        T¤TAL=0.
C
C       READ INPUT AND ALPHA IDENTIFICATI¤N CARD
        READ102
        PUNCH102
        PUNCH103
        READ 114,(U(I),I=1,9)
        PUNCH115,(U(I),I=1,9)
      1 READ101,A,B,DELTA1,JMAX
C
C       TEST INPUT F¤R VALIDITY, IF ¤KAY PUNCH NEXT PART ¤F ¤UTPUT
        IF(JMAX-2)26,26,27
     26 IF(N)25,25,29
     25 PUNCH106
        ST¤P
     27 IF(B-A)22,28,22
     28 PUNCH104
        ST¤P
     22 IF(DELTA1)23,24,23
     24 PUNCH105
        ST¤P
     23 PUNCH109,B,JMAX
        PUNCH110,A,DELTA1
C
C       INITIALIZATI¤N F¤R START
        C¤UNT=0.
        SUM=0.
        SUMFX=0.
        N=N+1
        J=1
        K2=2
     21 DELX=(B-A)/(2.**J)
        IF(J-1)4,2,4
      2 D¤ 3I=1,3
        AI=I-1
        X= A+ AI*DELX
        F(I)=FUN(X)
        SUM = SUM+Q(I)*F(I)
      3 SUMFX=SUMFX+P(I)*F(I)
C       FIRST APPR¤XIMATI¤N ¤F INTEGRAL
        AN1=DELX*SUMFX/3.
        J=J+1
```

```
      GO TO 21
C     CALCULATES FUNCTION MIDWAY BETWEEN CURRENT POINTS
    4 SUMFX=0.
      DO 5 I=1,K2
      AT = 2*I-1
      X= A+AT*DELX
    5 SUMFX = SUMFX+FUN(X)
C     NEXT APPROXIMATION
      AN2=DELX*(4.*SUMFX+SUM )/3.
      IF(AN2)6,12,6
    6 DELTA=ABSF((AN1-AN2)/AN2*100.)
      IF(DELTA-DELTA1)17,17,18
   18 IF(J-JMAX)19,17,17
   19 AN1=AN2
      SUM =SUM +2.*SUMFX
      PUNCH112,J,AN1,DELTA
C     INITIALIZATION FOR NEXT ITERATION  LOOP
      J=J+1
      K2=2*K2
C     BACK TO ITERATION  IF VALUE HAS NOT CONVERGED ENOUGH
      GO TO 21
C
C     PUNCH FINAL ANSWER FOR THIS PASS AND RETURN FOR NEXT INPUT CARD
   17 PUNCH 113,J,N,AN2,DELTA
      TOTAL =TOTAL+AN2
      GO TO 1
C
C     FOR HANDLING ZERO ANSWERS
   12 COUNT=COUNT+1.
      IF(COUNT-2.)18,17,17
C
C     PUNCH THE TOTAL ANSWER AND HALT
   29 PUNCH116,N,TOTAL
      STOP
  101 FORMAT(2F12.6,F4.4,I2)
  102 FORMAT(80H
     1                                        )
  103 FORMAT(/15X,48HNUMIT ONE  (ONE-DIM. INTEGRATION, SIMPSONS RULE)  )
  104 FORMAT(15X,17HCHECK INPUT - A=B)
  105 FORMAT(15X,22HCHECK INPUT - DELTA1=0)
  106 FORMAT(15X,32HCHECK INPUT - JMAX OUTSIDE RANGE)
  109 FORMAT(35X,10HINPUT DATA/20X,2HA=F12.6,11X,7HJ(MAX)=,I2)
  110 FORMAT(20X,2HA=,F12.6,11X,7HDELTA1=,F10.4//15X,10H ITERATION,11X,
     18HINTEGRAL,13X,5HDELTA)
  112 FORMAT(19X,I2,12X,F12.6,10X,F8.3)
  113 FORMAT(19X,I2,5H(PASS,I3,1H),3X,F12.6,10X,F8.3////)
  114 FORMAT(9A5)
  115 FORMAT(15X,7HF(X) = ,9A5,//)
  116 FORMAT(32X,12HNO. PASSES =I3/29X,16HTOTAL INTEGRAL = F12.5/39X,
     13HEND)
      END
```

APPENDIX C

Test Cases

Running time is still highly variable, but in general the time is now 30 to 50 percent faster than in the old version as will be noted in the test cases. Also, accuracy has been increased since quantities are now held to 10 significant figures.

Note the integrands of Cases 3(a) and 3(b) are identical to Case 2 and taken together duplicate Case 2. However, Case 3 produced a more accurate answer in a small fraction of the time for Case 2 because the Case 2 integral took on positive and negative values during the iteration attempting to approximate a zero answer while Case 3 integrated nonzero portions and summed them.

Running time, as in the original report, is still dependent on the formula

$$t = K \cdot 2^{J_{act}}$$

Table I gives the new running times for the test cases.

TABLE I

Test #	Integrand	a	b	J_{act}	t	$\frac{t\ new}{t\ old} \times 100$	K (min)
1	$\sqrt{(1-x^2)(2-x)}$	-1	1	11	12'50"	51.5	6.27×10^{-3}
2	sin(x)	0	2Π	11	16'50"	64.9	8.22×10^{-3}
3(a)	sin(x)	0	Π	5	1'	-	8.22×10^{-3}
3(b)	sin(x)	Π	2Π	5	1'	-	8.22×10^{-3}

TEST CASE 1

INPUT DATA

SOURCE STATEMENT OF SUBROUTINE

```
*1010
          FUNCTI¤N FUN(X)
          FUN =SQRTF((1.-X*X)*(2.-X))
          RETURN
          END
```

OUTPUT DATA

```
                         TEST FUNCTION 1

NUMIT ONE   %ONE-DIM. INTEGRATION, SIMPSONS RULE¤
F%X¤ #   SQRT%%1.-X*X¤%2.-X¤¤


                         INPUT DATA
     B# .100000E&01                    J%MAX¤#13
     A#-.100000E&01                    DELTA1# .1000E-02

  ITERATION                INTEGRAL                  DELTA
       2                  .209138E&01                 9.838
       3                  .216390E&01                 3.351
       4                  .218943E&01                 1.166
       5                  .219843E&01                  .409
       6                  .220161E&01                  .144
       7                  .220273E&01                  .050
       8                  .220312E&01                  .017
       9                  .220326E&01                  .006
      10                  .220331E&01                  .002
      11%PASS   1¤        .220333E&01                 0.000


                    NO. PASSES #   1
                TOTAL INTEGRAL # 2.20333E-00
                         END
```

TEST CASE 2

INPUT DATA

SOURCE STATEMENT OF SUBROUTINE

```
*1010
      FUNCTI¤N FUN(X)
      FUN  = SINF(X)
      RETURN
      END
```

OUTPUT DATA

```
                            TFST FUNCTION 2

   NUMIT ONE  %ONE-DIM. INTEGRATION, SIMPSONS RULE¤
   F%X¤ #  SIN%X¤

                            INPUT DATA
       B# .628319F&01                 J%MAX¤#11
       A# .000000F-99                 DELTA1# .1000E-02

    ITERATION             INTEGRAL                DELTA
        3              -.628319E-09              100.000
        4              -.523599E-09               20.000
        5               .641408E-09              181.632
        6              -.615229E-09              204.255
        7              -.187841E-08               67.247
        8              -.144971E-08               29.571
        9               .397608E-09              464.609
       10              -.443300E-08              108.969
       11%PASS  1¤     -.274807E-08               61.312

                         NO. PASSES #   1
                      TOTAL INTEGRAL #-2.74807E-09
                               END
```

TEST CASES 3(a) and 3(b)

OUTPUT DATA

TEST FUNCTIONS 3(a) and 3(b)

```
NUMIT ONE  %ONE-DIM. INTEGRATION, SIMPSONS RULE¤
F%X¤ #  SIN%X¤


                      INPUT DATA
    B# .314159E&01             J%MAX¤#11
    A# .000000E-99             DELTA1# .1000E-02

  ITERATION            INTEGRAL               DELTA
    2                .200455E&01             4.481
    3                .200026E&01              .214
    4                .200001E&01              .012
    5%PASS  1¤       .200000E&01             0.000



                      INPUT DATA
    B# .628319E&01             J%MAX¤#11
    A# .314159E&01             DELTA1# .1000E-02

  ITERATION            INTEGRAL               DELTA
    2               -.200455E&01             4.481
    3               -.200026E&01              .214
    4               -.200001E&01              .012
    5%PASS  2¤      -.200000E&01             0.000



                NO. PASSES #  2
            TOTAL INTEGRAL # 0.00000E-99
                       END
```

APPENDIX D

Glossary

$F_J(a,b)$	--	the approximation of the integral for the Jth iteration over the interval (a, b)
Δx_J	--	the mesh interval for the Jth iteration
$f(x)$	--	the integrand
C_J	--	the sum of the values of the integrand over the interval (a, b) whose coefficients are 2
D_J	--	the sum of the values of the integrand over the interval (a, b) whose coefficients are 4
J	--	used to denote iteration number
Δ_J	--	convergence number calculated for the Jth iteration
Δ	--	input convergence criterion number
a	--	beginning point of the integration interval
b	--	end point of the integration interval
m	--	used as an index in summation
J_{max}	--	maximum number of iterations permitted
J_{act}	--	actual number of iterations
K	--	constant used in estimating running time

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